

An extrapolation cascadic multigrid method combined with a fourth-order compact scheme for 3D Poisson equation

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Abstract Extrapolation cascadic multigrid (EXCMG) method is an efficient multigrid method which has mainly been used for solving the two-dimensional elliptic boundary value problems with linear finite element discretization in the existing literature. In this paper, we develop an EXCMG method to solve the three-dimensional Poisson equation on rectangular domains by using the compact finite difference (FD) method with unequal meshsizes in different coordinate directions. The resulting linear system from compact FD discretization is solved by the conjugate gradient (CG) method with a relative residual stopping criterion. By combining the Richardson extrapolation and tri-quartic Lagrange interpolation for the numerical solutions from two-level of grids (current and previous grids), we are able to produce an extremely accurate approximation of the actual numerical solution on the next finer grid, which can greatly reduce the number of relaxation sweeps needed. Additionally, a simple method based on the midpoint extrapolation formula is used for the fourth-order FD solutions on two-level of grids to achieve sixth-order accuracy on the entire fine grid cheaply and directly. The gradient of the numerical solution can also be easily obtained through solving a series of tridiagonal linear systems resulting from the fourth-order compact FD discretizations. Numerical results show that our EXCMG method is much more efficient than the classical V-cycle and W-cycle multigrid methods. Moreover, only few CG iterations are required on the finest grid to achieve full fourth-order accuracy in both the L^2 -norm and L^∞ -norm for the solution and its gradient when the exact solution belongs to C^6 . Finally, numerical result shows that our EXCMG method is still effective when the exact solution has a lower regularity, which widens the scope of applicability of our EXCMG method.

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1 Introduction

Poisson equation is a partial differential equation of elliptic type with broad application in electrostatics, mechanical engineering, theoretical physics and geophysics. The Dirichlet boundary value problem for the three-dimensional (3D) Poisson equation has the following form:

$$\begin{cases} u_{xx} + u_{yy} + u_{zz} = f(x, y, z), & \text{in } \Omega, \\ u(x, y, z) = g(x, y, z), & \text{on } \partial\Omega, \end{cases} \quad (1)$$

where Ω is a 3D rectangle domain and $\partial\Omega$ is its boundary. Here we assume that the forcing function $f(x, y, z)$, the boundary function $g(x, y, z)$ and the exact solution $u(x, y, z)$ are continuously differentiable and have the necessary continuous partial derivatives up to certain orders.

The compact finite difference (FD) method for solving Poisson equations has been well studied since 1984 [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. Specifically, two-dimensional (2D) and 3D Poisson equations can be solved by high-order compact FD methods [1, 2, 3, 4, 5, 6]. These schemes are called “compact” since they only use minimum grid points to achieve fourth-order accuracy explicitly in the discretization formulas. Moreover, there has been a renewed interest in combining high-order compact scheme with multigrid method to solve Poisson equations. The classical multigrid method [14, 15, 16] combined with compact FD method for solving 2D and 3D Poisson equations has been conducted in [7, 8, 9, 10, 11, 12, 13, 17]. For example, Wang and Zhang [11] proposed a Richardson extrapolation for the numerical solutions from the two-level grids together with an operator based interpolation iterative strategy to achieve sixth-order accuracy by using the classical multigrid method and the fourth-order compact FD scheme. Ge [13] developed a fourth-order compact FD method with the classical multigrid method to solve the 3D Poisson equation using unequal meshsizes in different coordinate directions. Dehghan et al. [17] solved the 1D, 2D and 3D Poisson equations with both second-order and fourth-order compact FD methods based on a new two-grid multigrid method. Besides Poisson equation, the classical multigrid method has been applied to many problems, including the biharmonic equation [18], the convection-diffusion equation [19, 20, 21] and so on.

Cascadic multigrid (CMG) method proposed by Deuffhard and Bornemann in [22] is a variant of the multigrid without any coarse grid correction steps, where instead of starting from the finest grid, the solution is first computed on the coarsest grid and the recursively interpolated and relaxed on finer grids. Bornemann and Deuffhard [22] showed that it is an optimal iteration method with respect to the energy norm. Since the 1990s, the method has been frequently used to solve the elliptic equation with the finite element (FE) discretization because of its high efficiency and simplicity [24, 25, 26, 27, 28, 29, 30, 31, 32]. In 2007, Shi et al. [35] proposed an economical cascadic multigrid method using the different criteria for choosing the smoothing steps on each level of grid. Later, based on a new Richardson extrapolation formula for the linear FE solution, an extrapolation cascadic multigrid (EXCMG) method was first proposed by Chen et al. [36, 37] to solve 2D Poisson equation with the linear FE discretization. For the EXCMG method, in order to obtain a better initial guess of the iterative solution on the next finer grid, numerical solutions on the two-level of grids (current

and previous grids) are needed (whereas only one-level of numerical solution is needed in the CMG method). The EXCMG algorithm has been successfully applied to non-smooth problems [38], linear parabolic problems [39], and the simulation of the electric field with a point singularity arising in geophysical exploration [40, 41]. However, to our best knowledge, the EXCMG algorithm has mainly been used for solving the 2D elliptic problems with the linear FE discretization in existing literature. But it is of more importance to solve the 3D problems efficiently and accurately arising in many engineering areas, such as geophysical exploration [42]. Since the construction process of the higher-order (at least fifth-order) approximation to the fourth-order compact FD solution on the next finer grid has to be different from the construction process of the third-order approximation to the second-order FE solution, it will be nontrivial to extend the EXCMG method from 2D problems with second-order FE discretization to 3D problems with fourth-order compact FD discretization.

In this paper, we will propose an EXCMG method combined with the fourth-order compact difference scheme to solve the Dirichlet boundary value problem of the 3D Poisson equation (1) in rectangular domains. In our approach, the computational domain is discretized by regular grids, and a 19-point fourth-order compact difference scheme is used to discretize the 3D Poisson equation with unequal meshsizes in different directions. By combining the Richardson extrapolation and tri-quartic Lagrange interpolation for the numerical solutions from two-level of grids (current and previous grids), we are able to obtain a much better initial guess of the iterative solution on the next finer grid than one obtained by using linear interpolation in CMG method. Then, the resulting large linear system is solved by the conjugate gradient (CG) solver using the above obtained initial guess. Additionally, a tolerance related to relative residual is introduced in the CG solver in order to obtain conveniently the numerical solution with the desired accuracy. Moreover, when the exact solution is sufficiently smooth, a simple method based on the midpoint extrapolation formula can be used to obtain cheaply and directly a sixth-order accurate solution on the entire fine grid from two fourth-order FD solutions on two different scale grids (current and previous grids). And a fourth-order compact FD scheme can be used to compute the gradient of the solution by solving a series of tridiagonal linear systems. Finally, our method has been used to solve 3D Poisson equations with more than 16 million unknowns in about 10 seconds on a desktop with 16GB RAM installed, which is much more efficient than the classical multigrid methods.

The rest of the paper is organized as follows: section 2 gives the description of the compact FD discretization for the 3D Poisson equation. Section 3 reviews the classical V-cycle and W-cycle multigrid methods. In section 4, we first derive some sixth-order extrapolation formulas, and then develop a new EXCMG method to solve 3D Poisson equation. Section 5 presents the numerical results to demonstrate the high efficiency and accuracy of the proposed method. And conclusions are given in the final section.

2 Compact difference scheme

We consider a cubic domain $\Omega = [0, L_x] \times [0, L_y] \times [0, L_z]$, and discretize the domain with unequal meshsizes h_x, h_y and h_z in the x, y and z coordinate directions, respectively. Let $N_x = L_x/h_x, N_y = L_y/h_y, N_z = L_z/h_z$ be the numbers of uniform intervals along the x, y and z directions. The grid points are (x_i, y_j, z_k) , with $x_i = ih_x, y_j = jh_y$ and $z_k = kh_z, i = 0, 1, \dots, N_x, j = 0, 1, \dots, N_y$ and $k = 0, 1, \dots, N_z$. The quantity $u_{i,j,k}$ represents the numerical solution at (x_i, y_j, z_k) .

Then the value on the boundary points $u_{i,j,k}$ ($i = 0, N_x$ or $j = 0, N_y$ or $k = 0, N_z$) can be evaluated directly from the Dirichlet boundary condition. For internal grid points ($i = 1, \dots, N_x - 1, j = 1, \dots, N_y - 1, k = 1, \dots, N_z - 1$), the 19-point fourth-order compact difference scheme with unequal-meshsize for 3D Poisson equation was derived in [6, 13]:

$$\begin{aligned}
& -8 \left(\frac{1}{h_x^2} + \frac{1}{h_y^2} + \frac{1}{h_z^2} \right) u_{i,j,k} + \left(\frac{4}{h_x^2} - \frac{1}{h_y^2} - \frac{1}{h_z^2} \right) (u_{i+1,j,k} + u_{i-1,j,k}) + \left(\frac{4}{h_y^2} - \frac{1}{h_x^2} - \frac{1}{h_z^2} \right) (u_{i,j+1,k} + u_{i,j-1,k}) \\
& + \left(\frac{4}{h_z^2} - \frac{1}{h_x^2} - \frac{1}{h_y^2} \right) (u_{i,j,k+1} + u_{i,j,k-1}) + \frac{1}{2} \left(\frac{1}{h_x^2} + \frac{1}{h_y^2} \right) (u_{i+1,j+1,k} + u_{i+1,j-1,k} + u_{i-1,j+1,k} + u_{i-1,j-1,k}) \\
& + \frac{1}{2} \left(\frac{1}{h_x^2} + \frac{1}{h_z^2} \right) (u_{i+1,j,k+1} + u_{i+1,j,k-1} + u_{i-1,j,k+1} + u_{i-1,j,k-1}) \\
& + \frac{1}{2} \left(\frac{1}{h_y^2} + \frac{1}{h_z^2} \right) (u_{i,j+1,k+1} + u_{i,j-1,k+1} + u_{i,j+1,k-1} + u_{i,j-1,k-1}) \\
& = \frac{1}{2} (6f_{i,j,k} + f_{i+1,j,k} + f_{i-1,j,k} + f_{i,j+1,k} + f_{i,j-1,k} + f_{i,j,k+1} + f_{i,j,k-1}).
\end{aligned} \tag{2}$$

Let $h = \max\{h_x, h_y, h_z\}$, throughout this paper, we denote u_h to be the FD solution of (2) with mesh sizes h_x, h_y, h_z , while use $u_{h/2}$ to denote the FD solution of (2) when mesh sizes are $h_x/2, h_y/2, h_z/2$. Then the difference scheme (2) can be expressed in the following matrix form:

$$A_h u_h = f_h, \tag{3}$$

where A_h is a sparse positive definite matrix, and f_h denotes the right hand-side vector of (2) with mesh sizes h_x, h_y and h_z .

3 Classical multigrid methods

The multigrid method is based on the idea that classical relaxation methods strongly damp the oscillatory error components, but converge slowly for smooth error components [15, 16]. Hence, after a few relaxation sweeps, we compute the smooth residual of the current approximation v_h (with mesh sizes h_x, h_y, h_z) and transfer it to a coarser grid \mathcal{Q}_{2h} (with mesh sizes $2h_x, 2h_y, 2h_z$) by a restriction operation, where the errors become more oscillatory. Solving the residual equation on the coarse grid \mathcal{Q}_{2h} , interpolating the correction back to the fine grid \mathcal{Q}_h , and adding it to the fine-grid current approximation v_h yields to the two-grid correction method. Since the coarse-grid problem is not much different from the original problem, we can perform a few, say γ , two-grid iteration steps (see Fig. 1) to the residual equation on the coarse grid, which means relaxing there and then moving to \mathcal{Q}_{4h} (with mesh sizes $4h_x, 4h_y, 4h_z$) for the correction step. We can repeat this process on successively coarser grids until a direct solution of the residual equation is possible. Then the corrections are interpolated back to finer grids until the process reaches the finest grid \mathcal{Q}_h (with mesh sizes h_x, h_y, h_z) and the fine-grid approximate solution is corrected.

Usually, the cases $\gamma = 1$ and $\gamma = 2$ are particularly interesting. We refer to the case $\gamma = 1$ as V-cycle and to $\gamma = 2$ as W-cycle. The number γ is also called cycle index. A V-cycle multigrid method is obtained when the V-cycle is repeated until a stopping criterion is satisfied on the finest grid. We refer to a V-cycle (W-cycle) with v_1 relaxation sweeps before the correction step and v_2 relaxation sweeps after the correction step as a $V(v_1, v_2)$ -cycle ($W(v_1, v_2)$ -cycle).

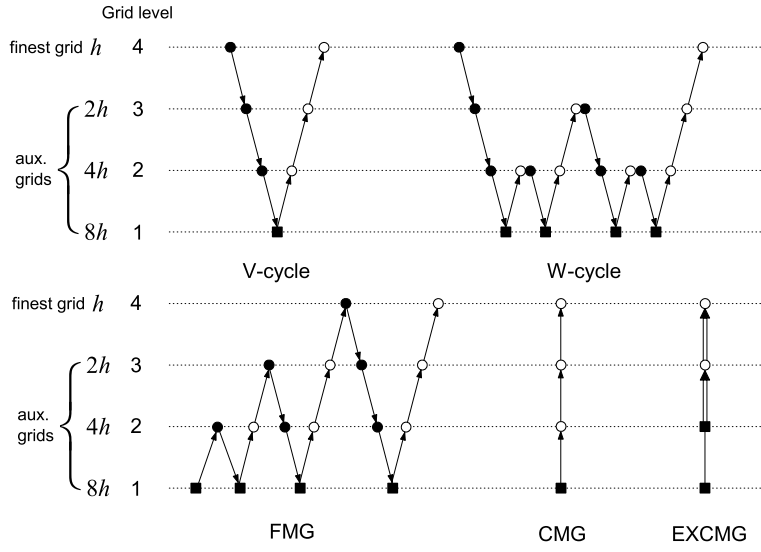


Fig. 1 The four-level structure of the V-cycle, W-cycle, FMG, CMG and EXCMG methods. In the diagram, ● denotes pre-smoothing, ○ denotes post-smoothing, ↑ denotes prolongation (usually defined by linear interpolation), ↓ denotes restriction, ⇑ denotes extrapolation and high-order interpolation, and ■ denotes direct solver.

4 Extrapolation cascadic multigrid methods

The CMG method proposed by Deufhard and Bornemann in [22] is a variant of full multigrid (FMG) method without any coarse grid correction steps but with an a posteriori control of the number of smoothing iterations (see Fig. 1). It has been shown that the CMG method has optimal computational complexity for both conforming and nonconforming elements with CG as a smoother. Since the 1990s, the CMG method has received quite a bit of attention from researchers because of its high efficiency and simplicity [23, 24, 25, 26, 27, 28, 29, 30].

In 2008, by using Richardson extrapolation and bilinear quadratic interpolation for the FE solutions on two-level of grids (current and previous grids) to obtain an extremely accurate initial guess of the iterative solution on the next finer grid, Chen et al. [36] proposed an extrapolation cascadic multigrid (EXCMG) method to solve 2D elliptic boundary value problems. It has been shown in [37] that the EXCMG method is much more efficient than the CMG method, which simply uses the linear interpolation for the FE solution on the current grid to provide an initial guess of the iterative solution on the next finer grid. Recently, we improved and generalized the EXCMG method to solve large linear systems resulting from FE discretization of 3D elliptic problems, compared it with the classical multigrid methods, and further presented the reason why EXCMG algorithms are highly efficient [44]. However, to our best knowledge, CMG and EXCMG are mainly used for linear FE method in existing literature, and it will be interesting to extend the EXCMG method to the field of high-order FD method.

4.1 EXCMG algorithm combined with compact difference scheme

The key ingredients of the EXCMG method are extrapolation and high-order interpolation (see Fig. 1), which can produce a much better initial guess of the iterative solution on the next finer grid than one obtained by using linear interpolation in CMG method.

In this subsection, we will propose a new EXCMG method combined with fourth-order compact difference scheme for solving the Dirichlet boundary value problem of the 3D Poisson equation, which is stated in the following algorithm.

Algorithm 1 New EXCMG method: $(u_h, \tilde{u}_h) \leftarrow \text{EXCMG}(A_h, f_h, L, \epsilon)$

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1:  $u_H \leftarrow \text{DSOLVE}(A_H u_H = f_H)$   $\triangleright u_H$  is FD solution of (3) with mesh sizes  $H_x, H_y, H_z$ .
2:  $u_{H/2} \leftarrow \text{DSOLVE}(A_{H/2} u_{H/2} = f_{H/2})$   $\triangleright u_{H/2}$  is FD solution of (3) with mesh sizes  $H_x/2, H_y/2, H_z/2$ .
3:  $h_x = H_x/2, h_y = H_y/2, h_z = H_z/2$ 
4: for  $i = 1$  to  $L$  do
5:    $h_x = h_x/2, h_y = h_y/2, h_z = h_z/2$ 
6:    $w_h = \text{EXP}_{\text{finite}}(u_{2h}, u_{4h})$   $\triangleright w_h$  is a fifth-order approximation of the actual numerical solution  $u_h$ , and it serves as the initial guess for the CG solver on the next finer grid.
7:   while  $\|A_h u_h - f_h\|_2 > \epsilon \cdot \|f_h\|_2$  do
8:      $u_h \leftarrow \text{CG}(A_h, u_h, f_h)$ 
9:   end while
10:   $\tilde{u}_h = \text{EXP}_{\text{true}}(u_h, u_{2h})$   $\triangleright$  Optional step.  $\tilde{u}_h$  is a sixth-order approximation solution for sufficiently smooth  $u$ .
11: end for
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In Algorithm 1, the coarsest grid has the mesh sizes H_x, H_y, H_z , the positive integer L is the total number of grids except first two embedded grids, which indicates that the mesh sizes of the finest grid are $\frac{H_x}{2^{L+1}}, \frac{H_y}{2^{L+1}}, \frac{H_z}{2^{L+1}}$. DSOLVE is a direct solver used on the first two coarse grids (see line 1-2 in Algorithm 1). Procedure $\text{EXP}_{\text{finite}}(u_{2h}, u_{4h})$ denotes a fifth-order approximation to the actual compact FD solution u_h obtained by Richardson extrapolation and tri-quartic Lagrange interpolation from the numerical solutions u_{2h} and u_{4h} . And there is an optional step in the above algorithm (see line 10 in Algorithm 1), where $\text{EXP}_{\text{true}}(u_h, u_{2h})$ denotes a higher-order approximation solution on entire fine grid with mesh size h from two fourth-order FD solutions u_h and u_{2h} . This optional step is used to increase the order of solution accuracy from fourth order to sixth order (see Table 1-10 in section 5 for details) when the exact solution u of elliptic equation (1) is sufficiently smooth.

The detailed procedures of extrapolation and tri-quartic Lagrange interpolation are described in the next two subsections 4.2 and 4.3. The differences between our new EXCMG method and existing EXCMG method [36, 37] are listed as follows:

- (1) In our new EXCMG method, a fourth-order compact difference scheme, rather than the second-order linear FE method, is employed to discretize the 3D Poisson equation.
- (2) Instead of performing a fixed number of smoothing iterations as used in the existing EXCMG method [36, 37], a relative residual tolerance ϵ is introduced for the smoother in our EXCMG method (see line 7 in Algorithm 1), which enables us to conveniently obtain the numerical solution with the desired accuracy.
- (3) In the existing EXCMG literature [36, 37], a third-order approximation to the second-order FE solution is constructed to serve as the initial guess for the iterative solver on the next finer grid, and the construction of the third-order approximation to the second-order FE solution is done at every single coarse hexahedral element. However, in our new EXCMG method, a fifth-order approximation to the fourth-order FD solution, obtained

through the Richardson extrapolation and tri-quartic Lagrange interpolation, is used as the initial guess for the iterative solver. In addition, the tri-quartic interpolation should be done for every cell which contains eight neighboring coarse hexahedral elements as shown in Fig. 3, rather than every single coarse hexahedral element.

4.2 Extrapolation and quartic interpolation: 1D case

The extrapolation method is an efficient procedure for increasing the solution accuracy of many problems in numerical analysis. Marchuk and Shaidurov [45] systematically studied its application in the FD method in 1983. Since then, this technique has been well demonstrated in the framework of the FD and FE methods [46, 47, 48, 21, 49, 50, 51, 52, 53, 54].

In this and next subsections, we assume that the exact solution u is sufficiently smooth, and we will formally explain how to use extrapolation and quartic interpolation techniques to obtain the fifth-order approximation w_h of the fourth-order FD solution on the next finer grid, which can be regarded as another important application of the extrapolation method. In addition, we will also show how to construct the enhanced sixth-order accurate numerical solution \tilde{u}_h for the problem (1).

4.2.1 Extrapolation for the true solution

For simplicity, we first consider the three-levels of embedded grids $Z_i (i = 0, 1, 2)$ with mesh sizes $h_i = h_0/2^i$ in one dimension. Suppose $u \in H^6(\Omega)$, from theorem 4.1 in [43] (taking $m = 2, s = 6$) and by using the result that $H^2(\Omega)$ can be continuously embedded into $L^\infty(\Omega)$, we can get that the error $\|e^i\|_\infty$ should be $O(h^4)$, where $e^i = u^i - u$ is the error of the fourth-order compact FD solution u^i with mesh size h_i . Now we further assume that the truncation error at node x_k has the form

$$e^i(x_k) = A(x_k)h_i^4 + O(h_i^6), \quad (4)$$

where $A(x)$ is a suitably smooth function independent of h_i . The truncation error expansion (4) will be verified by numerical results in section 5.

It is well known that the traditional extrapolation is possible only at coarse grid points, where at least two approximations, corresponding to different mesh size, are known. From eq. (4), we easily obtain the Richardson extrapolation formula at coarse grid points

$$\tilde{u}_k^1 := \frac{16u_k^1 - u_k^0}{15} = u(x_k) + O(h_0^6), \quad k = j, j+1, \quad (5)$$

which is a sixth-order approximation to the true solution at the coarse grid points.

In fact, by using the linear interpolation formula, one can also obtain a sixth-order accurate approximation at the fine grid point $x_{j+1/2}$. Setting $i = 0$ and $i = 1$ in eq. (4) and then subtracting each other, we have

$$A(x_k) = \frac{16}{15h_0^4}(u_k^0 - u_k^1) + O(h_0^2), \quad k = j, j+1. \quad (6)$$

From the error estimate of the linear interpolation

$$A(x_{j+1/2}) = \frac{1}{2}(A(x_j) + A(x_{j+1})) + O(h_0^2), \quad (7)$$

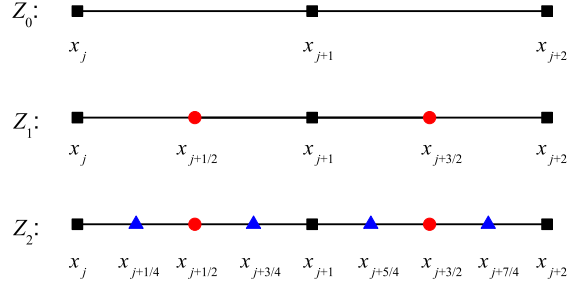


Fig. 2 Three embedded grids for two neighboring coarse elements in 1D.

and substituting eq. (6) into eq. (7), we get

$$A(x_{j+1/2}) = \frac{8}{15h_0^4}(u_j^0 - u_j^1) + \frac{8}{15h_0^4}(u_{j+1}^0 - u_{j+1}^1) + O(h_0^6). \quad (8)$$

Since

$$u_{j+1/2}^1 = u(x_{j+1/2}) + \frac{1}{16}A(x_{j+1/2})h_0^4 + O(h_0^6), \quad (9)$$

by using (8), we obtain the following midpoint extrapolation formula:

$$\tilde{u}_{j+1/2}^1 := u_{j+1/2}^1 + \frac{1}{30}(u_j^1 - u_j^0 + u_{j+1}^1 - u_{j+1}^0) = u(x_{j+1/2}) + O(h_0^6), \quad (10)$$

which is a sixth-order approximation to the true solution at the fine grid point $x_{j+1/2}$.

4.2.2 Extrapolation for the FD solution

In this part, we will explain, given the fourth-order FD solutions u^0 and u^1 , how to use the extrapolation and high-order interpolation techniques to construct a fifth-order (to be illustrated in subsection 4.4) approximation w^2 to the FD solution u^2 .

Adding one midpoint and two four equal division points, the coarse mesh element (x_j, x_{j+1}) is uniformly refined into four elements of fine mesh Z_2 as shown in Fig. 2. Assume there exists a constant c such that

$$cu^1 + (1 - c)u^0 = u^2 + O(h_0^6). \quad (11)$$

Here, we aim to use a linear combination of u^0 and u^1 to approximate the FD solution u^2 up to sixth-order accuracy. Substituting the asymptotic error expansion (4) into (11), we obtain $c = 17/16$ and an extrapolation formula

$$w_k^2 := \frac{17u_k^1 - u_k^0}{16} = u_k^2 + O(h_0^6), \quad k = j, j+1, \quad (12)$$

at nodes x_j and x_{j+1} . To derive the extrapolation formula at midpoint $x_{j+1/2}$, eq. (4) leads to

$$u_{j+1/2}^2 = u_{j+1/2}^1 - \frac{15}{256}A(x_{j+1/2})h_0^4 + O(h_0^6). \quad (13)$$

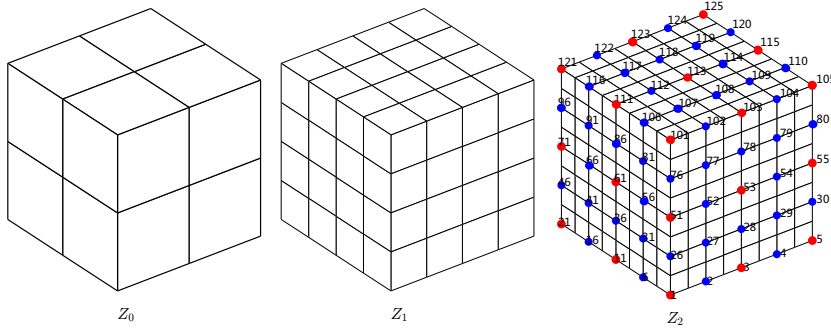


Fig. 3 Three embedded grids on one interpolation cell which contains eight neighboring coarse hexahedral elements.

Substituting eq. (8) into eq. (13), we have the following sixth-order extrapolation formula at the midpoint $x_{j+1/2}$,

$$w_{j+1/2}^2 := u_{j+1/2}^1 + \frac{1}{32}(u_j^1 - u_j^0 + u_{j+1}^1 - u_{j+1}^0) = u_{j+1/2}^2 + O(h_0^6). \quad (14)$$

Sixth-order extrapolation formulas (12) and (14) can be efficiently applied to each coarse-grid element (x_j, x_{j+1}) .

Once the five approximated values $w_j^2, w_{j+1/2}^2, w_{j+1}^2, w_{j+3/2}^2$ and w_{j+2}^2 are obtained on the two neighboring coarse elements, we can get the following four equal division point extrapolation formulas by using the quartic interpolation

$$w_{j+1/4}^2 := \frac{1}{128}(35w_j^2 + 140w_{j+1/2}^2 - 70w_{j+1}^2 + 28w_{j+3/2}^2 - 5w_{j+2}^2), \quad (15)$$

$$w_{j+3/4}^2 := \frac{1}{128}(-5w_j^2 + 60w_{j+1/2}^2 + 90w_{j+1}^2 - 20w_{j+3/2}^2 + 3w_{j+2}^2), \quad (16)$$

$$w_{j+5/4}^2 := \frac{1}{128}(-5w_j^2 + 28w_{j+1/2}^2 - 70w_{j+1}^2 + 140w_{j+3/2}^2 + 35w_{j+2}^2), \quad (17)$$

$$w_{j+7/4}^2 := \frac{1}{128}(3w_j^2 - 20w_{j+1/2}^2 + 90w_{j+1}^2 + 60w_{j+3/2}^2 - 5w_{j+2}^2). \quad (18)$$

Until now, we have obtained a high-order approximation w^2 to the FD solution u^2 , which can be used as the initial guess of the iterative solution on the fine mesh Z_2 .

4.3 Extrapolation and quartic interpolation: 3D case

In this subsection, we explain how to obtain a fifth-order accurate approximation w^2 to the fourth-order FD solution u^2 , and a sixth-order accurate approximate solution \tilde{u}^1 to the problem (1) for embedded hexahedral grids as shown in Fig. 3.

Taking every interpolation cell which consists of eight neighboring coarse hexahedral elements (see Fig. 3) into account, the construction processes of the approximation w^2 are as follows:

Corner Nodes (such as 1, 3, 51, 53): The approximate values at 27 corner nodes ‘●’ on such interpolation cell can be obtained by using the extrapolation formula (12).

Midpoints of edges (such as 2, 6, 26, 28): The approximate values at these 54 midpoints ‘●’ on such interpolation cell can be obtained by using the midpoint extrapolation formula (14) in x -direction, y -direction or z -direction.

Centers of faces (such as 27, 31, 107, 109): Since the center of each face on such interpolation cell can be viewed as the midpoint of two face diagonals, using the midpoint extrapolation formula (14) we can obtain two approximate values, and take the arithmetic mean as the approximation at these 36 midpoints ‘●’.

Centers of coarse hexahedral elements (such as 32, 42, 82, 92): Since the center of each coarse hexahedral element on such interpolation cell can be viewed as the midpoint of four space diagonals, again using the midpoint extrapolation formula (14) we can obtain four approximate values, and take the arithmetic mean as the approximation at these 8 midpoints ‘●’.

Other fine grid points: The approximate values of remaining $604(9^3 - 5^3)$ fine grid points on such the interpolation cell can be obtained by using tri-quartic Lagrange interpolation with the known 125-node (27 corner nodes, 54 midpoints of edges, 36 centers of faces and 8 centers of coarse hexahedral elements) values.

The tri-quartic Lagrange interpolation function in terms of natural coordinates (ξ, η, ζ) is

$$w^2(\xi, \eta, \zeta) = \sum_{m=1}^{125} N_m(\xi, \eta, \zeta) w_m^2, \quad (19)$$

where the shape functions N_m can be written as follows

$$N_m(\xi, \eta, \zeta) = l_i^4(\xi) l_j^4(\eta) l_k^4(\zeta), \quad (20)$$

where $l_i^4(x)$ ($0 \leq i \leq 4$) is the Lagrange fundamental polynomials of degree 4, defined as

$$l_i^4(\xi) = \prod_{k=0, k \neq i}^4 \frac{\xi - \xi_k}{\xi_i - \xi_k}, \quad (21)$$

and (ξ_i, η_j, ζ_k) is the natural coordinate of node m ($1 \leq m \leq 125$).

When constructing the sixth-order accurate solution \tilde{u}^1 based on two fourth-order accurate solutions u^0 and u^1 , the Richardson extrapolation formula (5) can be directly used for coarse grid points, while the sixth-order midpoint extrapolation formula (10) can be directly used for all other fine grid points, which is similar to the process (excluding the tri-quartic interpolation) of constructing the approximation w^2 described as above.

Remark 1 Since the compact FD solution u_h of (2) is a fourth-order approximation of the exact solution u , in order to get a quite good initial guess w_h for the CG solver, a tri-quartic Lagrange interpolation method is employed in this paper so that a fifth-order approximation of w_h to u_h is achieved. Moreover, the relative effect of how w_h approximates u_h becomes better when mesh is refined, thus, the number of iterations will be reduced most significantly on the finest grid, which is particularly important for solving large linear systems and can greatly reduce the computational cost. We note that the tri-quadratic interpolation used in [44] produces a third-order approximation to the second-order FE solution, and the tri-quadratic interpolation is accurate enough in that case. However, when u_h is obtained from the fourth-order compact FD method as shown in this paper, the tri-quadratic interpolation can not provide a sufficiently accurate initial guess w_h , the relative effect of how w_h approximates u_h will become worse when mesh is refined.

Remark 2 Tri-quartic Lagrange interpolation defined by eq. (19) is a local operation defining on each interpolation cell containing eight neighbouring coarse elements. In fact, eq. (19) defines a same (604×125) interpolation matrix on every interpolation cell, thus the approximate values of remaining $604(9^3 - 5^3)$ fine-grid points on every interpolation cell can be obtained by multiplying the (604×125) interpolation matrix with the vector consisting of 125 known values on such interpolation cell. Therefore, the fifth-order approximation of FD solution w_h on the entire domain can be obtained very effectively by applying the extrapolation formulas (12) and (14) to the 125 nodes mentioned above, and running the tri-quartic Lagrange interpolation (19) based on such 125 known values for every interpolation cell in the entire domain.

4.4 The error analysis of initial guess w^2

Let $e = w^2 - u^2$ be the difference between the initial guess w^2 and the FD solution u^2 . Assume that e has continuous derivatives up to order 5 on interval $[x_j, x_{j+2}]$. From (12) and (14) we obtain the equation

$$e(x_k) = O(h_0^6), \quad k = j, j + 1/2, j + 1, j + 3/2, j + 2. \quad (22)$$

From polynomial interpolation theory, the error of quartic interpolation $I_4 f$ can be represented as

$$R_4(x) = e - I_4 e = \frac{1}{5!} e^{(5)}(\xi)(x - x_j)(x - x_{j+1/2})(x - x_{j+1})(x - x_{j+3/2})(x - x_{j+2}), \quad (23)$$

where $\xi \in (x_j, x_{j+2})$ depends on x . Especially at four equal division points we have

$$R_4(x_{j+1/4}) = \frac{7h_0^5}{8 \times 4^5} e^{(5)}(\xi_1) = \frac{7h_0^5}{8192} e^{(5)}(x_{j+1}) + o(h_0^5), \quad (24)$$

$$R_4(x_{j+3/4}) = -\frac{3h_0^5}{8 \times 4^5} e^{(5)}(\xi_2) = -\frac{3h_0^5}{8192} e^{(5)}(x_{j+1}) + o(h_0^5), \quad (25)$$

and

$$R_4(x_{j+5/4}) = \frac{3h_0^5}{8 \times 4^5} e^{(5)}(\xi_3) = \frac{3h_0^5}{8192} e^{(5)}(x_{j+1}) + o(h_0^5) \approx -R_4(x_{j+3/4}), \quad (26)$$

$$R_4(x_{j+7/4}) = -\frac{7h_0^5}{8 \times 4^5} e^{(5)}(\xi_4) = -\frac{7h_0^5}{8192} e^{(5)}(x_{j+1}) + o(h_0^5) \approx -R_4(x_{j+1/4}). \quad (27)$$

It follows from eqs. (22) and (24)-(27) that

$$e(x_k) = I_4 e(x_k) + R_4(x_k) = O(h_0^5), \quad k = j + 1/4, j + 3/4, j + 5/4, j + 7/4, \quad (28)$$

which means that the initial guess w^2 obtained by extrapolation and quartic interpolation is a fifth-order accurate approximation to the FD solution u^2 .

The above error analysis can be directly extended to 3D case (see numerical verification in Section 5: the last columns in Table 1-11). In addition, eqs.(26) and (27) imply that the initial error $e(x)$ forms a high-frequency oscillation in the entire domain, however, it can be smoothed out after a few CG iterations (see Fig. 4 for details).

5 Numerical experiments

In this section, in order to illustrate the efficiency of the new EXCMG method comparing to the classical V-cycle and W-cycle multigrid methods with the Gauss-Seidel relaxation and the CG relaxation, we present the numerical results for six examples with smooth and finite regular solutions using the proposed method. Our code is written in Fortran 90 with double precision arithmetic, and compiled with Intel Visual Fortran Compiler XE 12.1 under 64-bit Windows 7. All programs are carried out on a personal desktop equipped with Intel(R) Core(TM) i7-4790K CPU (4.00 GHz) and 16GB RAM.

The order of convergence of the method is computed by

$$\text{order} = \log_2 \frac{\|u_h - u\|}{\|u_{h/2} - u\|}, \quad (29)$$

where $\|\cdot\|$ denotes some norm (for instance, L^2 -norm or L^∞ -norm) and u is the true solution.

5.1 Numerical accuracy

Example 1 The test Problem 1 can be written as

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = e^z \sin(xy)(1 - x^2 - y^2), \quad \text{in } \Omega = [0, 1]^3, \quad (30)$$

where the boundary conditions are

$$u(0, y, z) = u(x, 0, z) = 0, \quad u(1, y, z) = e^z \sin(y), \quad u(x, 1, z) = e^z \sin(x),$$

and

$$u(x, y, 0) = \sin(xy), \quad u(x, y, 1) = e \sin(xy).$$

The analytic solution of eq. (30) is

$$u(x, y, z) = e^z \sin(xy),$$

which is a sufficiently smooth function.

Using 7 embedded grids with the coarsest grid $4 \times 4 \times 4$, we present the numerical results for Problem 1 obtained by the new EXCMG method with $\epsilon = 10^{-14}$ in Table 1-2. Table 1 lists the L^2 -error of the compact FD solution u_h , the L^2 -error of the gradient of the FD solution ∇u_h , the L^2 -error of the extrapolated solution \tilde{u}_h , the L^2 -norm of the difference between the initial guess w_h and the FD solution u_h , and corresponding convergence rates. Table 2 gives all errors and convergence rates in L^∞ -norm. Since a direct solver is used for the first two coarse levels of grids, we only list the results starting from the third level of grid $16 \times 16 \times 16$.

Here we explain how to numerically compute the gradient ∇u_h after we obtain the FD solution u_h . First, we use the following fourth-order, one-sided, FD approximation of the partial derivative u_x on the boundary grid points,

$$(u_x)_{0,j,k} = -\frac{25}{12h_x}u_{0,j,k} + \frac{4}{h_x}u_{1,j,k} - \frac{3}{h_x}u_{2,j,k} + \frac{4}{3h_x}u_{3,j,k} - \frac{1}{4h_x}u_{4,j,k}, \quad \text{for } j = 0, \dots, N_y, k = 0, \dots, N_z,$$

$$(u_x)_{N_x,j,k} = \frac{25}{12h_x}u_{N_x,j,k} - \frac{4}{h_x}u_{N_x-1,j,k} + \frac{3}{h_x}u_{N_x-2,j,k} - \frac{4}{3h_x}u_{N_x-3,j,k} + \frac{1}{4h_x}u_{N_x-4,j,k}, \quad \text{for } j = 0, \dots, N_y, k = 0, \dots, N_z.$$

Table 1 Errors and convergence rates with $\epsilon = 10^{-14}$ in L^2 -norm for Example 1.

mesh	$\ u_h - u\ _2$	order	$\ \nabla(u_h - u)\ _2$	order	$\ \tilde{u}_h - u\ _2$	order	$\ w_h - u_h\ _2$	order
$16 \times 16 \times 16$	1.67(-08)		1.08(-06)		1.38(-09)		4.36(-07)	
$32 \times 32 \times 32$	1.09(-09)	3.93	4.74(-08)	4.51	2.40(-11)	5.84	1.29(-08)	5.08
$64 \times 64 \times 64$	7.00(-11)	3.97	2.12(-09)	4.48	3.91(-13)	5.94	3.94(-10)	5.04
$128 \times 128 \times 128$	4.42(-12)	3.98	9.70(-11)	4.45	6.22(-15)	5.98	1.22(-11)	5.02
$256 \times 256 \times 256$	2.82(-13)	3.97	4.62(-12)	4.39	5.68(-15)	0.13	3.79(-13)	5.01

Table 2 Errors and convergence rates with $\epsilon = 10^{-14}$ in L^∞ -norm for Example 1.

mesh	$\ u_h - u\ _\infty$	order	$\ \nabla(u_h - u)\ _\infty$	order	$\ \tilde{u}_h - u\ _\infty$	order	$\ w_h - u_h\ _\infty$	order
$16 \times 16 \times 16$	5.47(-08)		8.25(-06)		9.12(-09)		3.85(-06)	
$32 \times 32 \times 32$	3.43(-09)	4.00	5.18(-07)	3.99	1.77(-10)	5.68	1.31(-07)	4.88
$64 \times 64 \times 64$	2.15(-10)	4.00	3.24(-08)	4.00	3.20(-12)	5.79	4.19(-09)	4.96
$128 \times 128 \times 128$	1.34(-11)	4.00	2.03(-09)	4.00	5.42(-14)	5.88	1.32(-10)	4.99
$256 \times 256 \times 256$	8.49(-13)	4.00	1.27(-10)	4.00	4.00(-14)	0.44	4.15(-12)	4.99

Then we can obtain $(u_x)_{i,j,k}$, $(i = 1, \dots, N_x - 1)$ on the internal grid points by solving the following linear system resulting from the fourth-order compact FD scheme [55],

$$\frac{1}{6}(u_x)_{i-1,j,k} + \frac{4}{6}(u_x)_{i,j,k} + \frac{1}{6}(u_x)_{i+1,j,k} = \frac{u_{i+1,j,k} - u_{i-1,j,k}}{2h_x}, \quad \text{for } j = 0, \dots, N_y, k = 0, \dots, N_z.$$

The above 1D tridiagonal system can be solved fast by the Thomas algorithm. Clearly, we can get u_y and u_z from similar procedures. Then, ∇u_h can be obtained efficiently.

As we can see from table 1-2 that initial guess w_h is a fifth-order approximation to the FD solution u_h , which validates our theoretical analysis in section 4.4, and the FD solution u_h achieves the full fourth-order accuracy. The numerical gradient ∇u_h is also a fourth-order approximation to the exact gradient ∇u in both the L^2 -norm and L^∞ -norm, while the extrapolated solution \tilde{u}_h converges with sixth-order accuracy on all grids except the finest grid. This is due to the fact that the extrapolated solution \tilde{u}_h is obtained from two fourth-order FD solutions u_h and u_{2h} , these two solutions must be extremely accurate in order to obtain a sixth-order accurate solution \tilde{u}_h . As the grid becomes finer, the relative residual tolerance needs to be smaller. Thus, the extrapolated solution \tilde{u}_h starts to lose convergence order when the grid is fine enough since a uniform tolerance is used in our EXCMG algorithm. And in this example, on the finest mesh $256 \times 256 \times 256$, the maximum error between the extrapolated solution \tilde{u}_h and the exact solution u already reaches $O(10^{-14})$, which is almost the machine accuracy, although the method does not achieve the full sixth-order on the finest grid. Additionally, we can see that the numerical results confirm with the asymptotic error expansion (4).

Example 2 The test Problem 2 can be written as

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0, \quad \text{in } \Omega = [0, 1]^3, \quad (31)$$

where the boundary conditions are

$$u(0, y, z) = e^y \sin(\sqrt{2}z), \quad u(x, 0, z) = e^x \sin(\sqrt{2}z), \quad u(x, y, 0) = 0,$$

and

$$u(1, y, z) = e^{1+y} \sin(\sqrt{2}z), \quad u(x, 1, z) = e^{x+1} \sin(\sqrt{2}z), \quad u(x, y, 1) = e^{x+y} \sin(\sqrt{2}).$$

Table 3 Errors and convergence rates with $\epsilon = 10^{-14}$ in L^2 -norm for Example 2.

mesh	$\ u_h - u\ _2$	order	$\ \nabla(u_h - u)\ _2$	order	$\ \tilde{u}_h - u\ _2$	order	$\ w_h - u_h\ _2$	order
$16 \times 16 \times 16$	4.26(-08)		150(-05)		2.28(-09)		6.21(-06)	
$32 \times 32 \times 32$	2.79(-09)	3.94	663(-07)	4.50	3.88(-11)	5.88	1.95(-07)	5.00
$64 \times 64 \times 64$	1.78(-10)	3.97	295(-08)	4.49	6.28(-13)	5.95	6.10(-09)	5.00
$128 \times 128 \times 128$	1.13(-11)	3.98	132(-09)	4.48	1.02(-14)	5.94	1.91(-10)	5.00
$256 \times 256 \times 256$	7.32(-13)	3.94	596(-11)	4.47	3.11(-14)	-1.60	5.97(-12)	5.00

Table 4 Errors and convergence rates with $\epsilon = 10^{-14}$ in L^∞ -norm for Example 2.

mesh	$\ u_h - u\ _\infty$	order	$\ \nabla(u_h - u)\ _\infty$	order	$\ \tilde{u}_h - u\ _\infty$	order	$\ w_h - u_h\ _\infty$	order
$16 \times 16 \times 16$	1.16(-07)		1.26(-4)		1.01(-08)		3.39(-05)	
$32 \times 32 \times 32$	7.22(-09)	4.00	7.95(-6)	3.99	1.86(-10)	5.76	1.11(-06)	4.94
$64 \times 64 \times 64$	4.52(-10)	4.00	4.98(-7)	4.00	3.17(-12)	5.87	3.54(-08)	4.96
$128 \times 128 \times 128$	2.83(-11)	4.00	3.11(-8)	4.00	5.95(-14)	5.74	1.12(-09)	4.99
$256 \times 256 \times 256$	1.81(-12)	3.96	1.95(-9)	4.00	1.07(-13)	-0.85	3.51(-11)	4.99

The analytic solution of eq. (31) is

$$u = e^{x+y} \sin(\sqrt{2}z),$$

which is a harmonic function and has arbitrary order smooth derivatives.

Again, we use 7 embedded grids with the coarsest grid $4 \times 4 \times 4$, and the corresponding numerical results obtained by the EXCMG method with $\epsilon = 10^{-14}$ are listed in table 3 and 4. Once again, initial guess w_h is a fifth-order approximation of the FD solution u_h , the FD solution u_h is fourth-order accurate, and the numerical gradient ∇u_h is also a fourth-order approximation to the exact gradient ∇u , while the extrapolated solution \tilde{u}_h converges to exact solution u with sixth-order but starts to lose accuracy on the finest grid $256 \times 256 \times 256$. Additionally, the maximum error between the extrapolated solution \tilde{u}_h and the exact solution u is less than 6.0×10^{-14} , which means that the solution \tilde{u}_h is already accurate enough, and we don't need to further reduce the error tolerance.

Example 3 The test Problem 3 can be written as

$$\begin{cases} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f(x, y, z), & \text{in } \Omega = [0, 1]^3, \\ u = g(x, y, z), & \text{on } \partial\Omega, \end{cases} \quad (32)$$

where f and g are determined from the exact solution

$$u = e^{-3((x-0.5)^2 + (y-0.5)^2 + (z-0.5)^2)},$$

which is a 3D Gaussian function. It varies rapidly near the point $(0.5, 0.5, 0.5)$.

Table 5 and 6 list the numerical results obtained by the EXCMG method with $\epsilon = 10^{-11}$. One more time, one can see that initial guess w_h is a fifth-order approximation of the FD solution u_h , the FD solution u_h is fourth-order accurate (although the convergent order is slightly reduced on the finest grid), and the numerical gradient ∇u_h is also a fourth-order approximation to the exact gradient ∇u , while the extrapolated solution \tilde{u}_h is sixth-order accurate. Therefore, our EXCMG method is still very effective for the problem with very rapid variations.

Table 5 Errors and convergence rates with $\epsilon = 10^{-11}$ in L^2 -norm for Example 3.

mesh	$\ u_h - u\ _2$	order	$\ \nabla(u_h - u)\ _2$	order	$\ \tilde{u}_h - u\ _2$	order	$\ w_h - u_h\ _2$	order
$16 \times 16 \times 16$	1.22(-06)		4.08(-04)		6.68(-08)		2.29(-04)	
$32 \times 32 \times 32$	7.90(-08)	3.95	1.29(-05)	4.99	1.15(-09)	5.86	5.80(-06)	5.30
$64 \times 64 \times 64$	5.04(-09)	3.97	4.42(-07)	4.86	1.87(-11)	5.94	1.86(-07)	4.96
$128 \times 128 \times 128$	3.19(-10)	3.98	1.73(-08)	4.67	3.05(-13)	5.94	5.86(-09)	4.99
$256 \times 256 \times 256$	2.40(-11)	3.73	7.50(-10)	4.53	4.52(-12)	-3.89	1.84(-10)	4.99

Table 6 Errors and convergence rates with $\epsilon = 10^{-11}$ in L^∞ -norm for Example 3.

mesh	$\ u_h - u\ _\infty$	order	$\ \nabla(u_h - u)\ _\infty$	order	$\ \tilde{u}_h - u\ _\infty$	order	$\ w_h - u_h\ _\infty$	order
$16 \times 16 \times 16$	4.80(-06)		1.03(-03)		2.14(-07)		1.13(-03)	
$32 \times 32 \times 32$	2.97(-07)	4.01	4.35(-05)	4.56	4.07(-09)	5.71	2.50(-05)	5.50
$64 \times 64 \times 64$	1.85(-08)	4.00	2.01(-06)	4.43	6.63(-11)	5.94	9.98(-07)	4.65
$128 \times 128 \times 128$	1.16(-09)	4.00	1.03(-07)	4.28	1.04(-12)	5.99	3.02(-08)	5.05
$256 \times 256 \times 256$	8.95(-11)	3.69	5.55(-09)	4.22	1.85(-11)	-4.15	9.27(-10)	5.03

Table 7 Errors and convergence rates with $\epsilon = 10^{-9}$ in L^2 -norm for Example 4.

mesh	$\ u_h - u\ _2$	order	$\ \nabla(u_h - u)\ _2$	order	$\ \tilde{u}_h - u\ _2$	order	$\ w_h - u_h\ _2$	order
$32 \times 16 \times 8$	3.58(-06)		2.85(-4)		4.55(-07)		7.86(-05)	
$64 \times 32 \times 16$	2.35(-07)	3.93	1.37(-5)	4.38	8.36(-09)	5.76	2.58(-06)	4.93
$128 \times 64 \times 32$	1.51(-08)	3.96	6.34(-7)	4.43	1.39(-10)	5.92	8.19(-08)	4.98
$256 \times 128 \times 64$	9.51(-10)	3.98	2.96(-8)	4.42	3.24(-12)	5.42	2.58(-09)	4.99
$512 \times 256 \times 128$	5.73(-11)	4.05	1.67(-9)	4.15	9.12(-12)	-1.49	7.99(-11)	5.01

Example 4 The test Problem 4 can be written as

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = -5.25\pi^2 \sin(2\pi x) \sin(\pi y) \sin\left(\frac{\pi}{2}z\right), \quad \text{in } \Omega = [0, 1]^3, \quad (33)$$

where the boundary conditions are

$$u(0, y, z) = u(1, y, z) = u(x, 0, z) = u(x, 1, z) = u(x, y, 0) = 0 \quad \text{and} \quad u(x, y, 1) = \sin(2\pi x) \sin(\pi y).$$

The analytic solution of eq. (33) is

$$u(x, y, z) = \sin(2\pi x) \sin(\pi y) \sin\left(\frac{\pi}{2}z\right),$$

which changes fastest in the x direction, faster in the y direction and slowest in the z direction.

Since the solution has the fastest change in the x -direction and the slowest change in the z -direction, we use the coarsest grid $8 \times 4 \times 2$ in the EXCMG algorithm. Table 7 and 8 list the numerical data obtained by EXCMG method using a tolerance $\epsilon = 10^{-9}$. Again, the initial guess w_h is a fifth-order approximation of the FD solution u_h , the FD solution u_h is fourth-order accurate, and the numerical gradient ∇u_h is also a fourth-order approximation to the exact gradient ∇u , while the extrapolated solution \tilde{u}_h achieves sixth-order accuracy but starts to lose accuracy on the finest grid since a uniform tolerance $\epsilon = 10^{-9}$ is used on each level of grid. The maximum error between the extrapolated solution \tilde{u}_h and the exact solution u already reaches $O(10^{-11})$ on the finest grid which is again quite accurate.

Previous examples are results for the 3D Poisson equation where the exact solution is infinitely many times continuously differentiable. In the following examples, we will show the results using the new EXCMG method for the cases where the exact solutions have finite regularities.

Table 8 Errors and convergence rates with $\epsilon = 10^{-9}$ in L^∞ -norm for Example 4.

mesh	$\ u_h - u\ _\infty$	order	$\ \nabla(u_h - u)\ _\infty$	order	$\ \tilde{u}_h - u\ _\infty$	order	$\ w_h - u_h\ _\infty$	order
$32 \times 16 \times 8$	1.10(-05)		1.78(-3)		2.74(-06)		3.58(-04)	
$64 \times 32 \times 16$	6.97(-07)	3.98	1.16(-4)	3.93	6.23(-08)	5.46	9.97(-06)	5.17
$128 \times 64 \times 32$	4.35(-08)	4.00	7.36(-6)	3.98	1.18(-09)	5.72	3.20(-07)	4.96
$256 \times 128 \times 64$	2.71(-09)	4.01	4.61(-7)	4.00	1.92(-11)	5.94	9.59(-09)	5.06
$512 \times 256 \times 128$	1.82(-10)	3.90	3.74(-8)	3.63	4.58(-11)	-1.26	2.82(-10)	5.09

Table 9 Errors and convergence rates with $\epsilon = 10^{-12}$ in L^2 -norm for Example 5.

mesh	$\ u_h - u\ _2$	order	$\ \nabla(u_h - u)\ _2$	order	$\ \tilde{u}_h - u\ _2$	order	$\ w_h - u_h\ _2$	order
$16 \times 16 \times 16$	5.44(-08)		1.22(-05)		3.35(-09)		2.32(-06)	
$32 \times 32 \times 32$	3.56(-09)	3.94	6.84(-07)	4.15	5.37(-11)	5.96	1.29(-07)	4.18
$64 \times 64 \times 64$	2.27(-10)	3.97	3.25(-08)	4.39	8.57(-13)	5.97	4.19(-09)	4.94
$128 \times 128 \times 128$	1.44(-11)	3.98	1.47(-09)	4.46	1.34(-14)	6.00	1.32(-10)	4.99
$256 \times 256 \times 256$	9.57(-13)	3.91	6.59(-11)	4.48	1.18(-13)	-3.14	4.12(-12)	5.00

Table 10 Errors and convergence rates with $\epsilon = 10^{-12}$ in L^∞ -norm for Example 5.

mesh	$\ u_h - u\ _\infty$	order	$\ \nabla(u_h - u)\ _\infty$	order	$\ \tilde{u}_h - u\ _\infty$	order	$\ w_h - u_h\ _\infty$	order
$16 \times 16 \times 16$	1.13(-07)		8.26(-5)		1.18(-08)		2.53(-05)	
$32 \times 32 \times 32$	7.16(-09)	3.98	5.83(-6)	3.82	2.08(-10)	5.83	6.96(-07)	5.18
$64 \times 64 \times 64$	4.48(-10)	4.00	3.76(-7)	3.96	3.32(-12)	5.97	2.48(-08)	4.81
$128 \times 128 \times 128$	2.80(-11)	4.00	2.36(-8)	3.99	5.25(-14)	5.98	8.02(-10)	4.95
$256 \times 256 \times 256$	1.81(-12)	3.95	1.50(-9)	3.97	2.58(-13)	-2.30	2.53(-11)	4.99

Example 5 The test Problem 5 can be written as

$$\begin{cases} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f(x, y, z), & \text{in } \Omega = [0, 1]^3, \\ u = g(x, y, z), & \text{on } \partial\Omega, \end{cases} \quad (34)$$

where $f(x, y, z)$ and $g(x, y, z)$ are determined from the exact solution

$$u = \frac{x^3 y^3 z^3}{(x^2 + y^2 + z^2)^{1.5}},$$

which has singularity at the origin and belongs to $H^{7.5-\epsilon}$ (ϵ is an arbitrary positive constant). It follows from the Sobolev embedding theorem that $u \in C^{6-\epsilon}$.

In the numerical computation, we also use 7 embedded grids with the coarsest grid $4 \times 4 \times 4$, and the corresponding numerical results by the EXCMG method with $\epsilon = 10^{-12}$ are listed in table 9 and 10. From table 9 and 10, one can easily find that the results are the same as previous examples, i.e., in both L^2 and L^∞ -norms, the initial guess w_h is a fifth-order approximation of the FD solution u_h , the FD solution u_h is fourth-order accurate, and the numerical gradient ∇u_h is also a fourth-order approximation to the exact gradient ∇u , while the extrapolated solution \tilde{u}_h achieves sixth-order accuracy but starts to lose accuracy on the finest grid since a uniform tolerance $\epsilon = 10^{-12}$ is used on each level of grid.

We further carry out the computations for other cases when the exact solution u has lower regularities, we find that if the exact solution $u \in H^s$ ($s < 7.5$), then the extrapolated solution \tilde{u}_h will not reach sixth-order accuracy in L^∞ -norm. In addition, we find that only when the exact solution u satisfies that $u \in H^s$ ($s \geq 5.5$), then the numerical solution u_h can reach fourth-order accuracy in L^∞ -norm. This is not surprising since $H^{7.5+\epsilon}(\Omega)$ can

Table 11 Errors and convergence rates with $\epsilon = 10^{-13}$ in L^2 -norm for Example 6.

mesh	$\ u_h - u\ _2$	order	$\ \nabla(u_h - u)\ _2$	order	$\ \tilde{u}_h - u\ _2$	order	$\ w_h - u_h\ _2$	order
$16 \times 16 \times 16$	2.39(-08)		7.11(-06)		2.68(-09)		1.54(-06)	
$32 \times 32 \times 32$	1.55(-09)	3.94	4.45(-07)	4.00	6.35(-11)	5.40	6.71(-08)	4.52
$64 \times 64 \times 64$	9.90(-11)	3.97	2.46(-08)	4.18	1.45(-12)	5.45	2.39(-09)	4.81
$128 \times 128 \times 128$	6.26(-12)	3.98	1.28(-09)	4.27	3.26(-14)	5.48	7.90(-11)	4.92
$256 \times 256 \times 256$	3.84(-13)	4.03	6.29(-11)	4.34	1.03(-13)	-1.66	2.54(-12)	4.96

Table 12 Errors and convergence rates with $\epsilon = 10^{-13}$ in L^∞ -norm for Example 6.

mesh	$\ u_h - u\ _\infty$	order	$\ \nabla(u_h - u)\ _\infty$	order	$\ \tilde{u}_h - u\ _\infty$	order	$\ w_h - u_h\ _\infty$	order
$16 \times 16 \times 16$	1.25(-07)		3.26(-5)		1.09(-07)		7.05(-06)	
$32 \times 32 \times 32$	7.81(-09)	4.00	4.08(-6)	3.00	6.82(-09)	3.50	4.40(-07)	4.00
$64 \times 64 \times 64$	4.88(-10)	4.00	5.10(-7)	3.00	4.26(-10)	3.50	2.75(-08)	4.00
$128 \times 128 \times 128$	3.05(-11)	4.00	6.38(-8)	3.00	2.67(-11)	3.50	1.72(-09)	4.00
$256 \times 256 \times 256$	2.04(-12)	3.90	7.92(-9)	3.01	3.71(-12)	3.61	1.08(-10)	4.00

be continuously embedding into $C^6(\Omega)$ and $H^{5.5+\epsilon}(\Omega)$ can be continuously embedding into $C^4(\Omega)$ from the Sobolev embedding theorem.

In the final part of this section, we will show the results for one example where the exact solution $u \in H^{5.5-\epsilon}$ (ϵ is an arbitrary small positive constant).

Example 6 The test Problem 6 can be written as

$$\begin{cases} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = \frac{8xyz}{(x^2 + y^2 + z^2)^{0.5}}, & \text{in } \Omega = [0, 1]^3, \\ u = g(x, y, z), & \text{on } \partial\Omega, \end{cases} \quad (35)$$

where eq. (35) has singularity at the origin and $g(x, y, z)$ is determined from the exact solution

$$u = xyz(x^2 + y^2 + z^2)^{0.5},$$

which belongs to $H^{5.5-\epsilon}$ (ϵ is an arbitrary small positive constant). It follows from the Sobolev embedding theorem that $u \in C^{4-\epsilon}$.

Once again, we use 7 embedded grids with the coarsest grid $4 \times 4 \times 4$, and the corresponding numerical results by the EXCMG method with $\epsilon = 10^{-13}$ are listed in table 11 and 12. Since in this case, the exact solution u is only has a finite regularity $H^{5.5-\epsilon}$ (ϵ is any positive constant). From table 11 and 12, we can see that the numerical solution u_h is a fourth-order approximation to the exact solution in both L^2 and L^∞ -norms. However, due to the lack of regularity of the exact solution, we can see from table 11 and 12 that the numerical gradient ∇u_h converges with fourth-order accuracy in L^2 -norm but only third-order in L^∞ -norm, the extrapolated solution \tilde{u}_h is 5.5th-order accurate in L^2 -norm but only 3.5th-order accurate in L^∞ -norm, while the initial guess w_h is only a fourth-order approximation to the FD solution u_h in L^∞ -norm. Nonetheless, the initial guess w_h is still a fifth-order approximation to the FD solution u_h in L^2 -norm. Since the relative residual in the CG solver in our new EXCMG method is calculated based on the L^2 -norm (see line 7 of the algorithm 1), thus, our EXCMG method is still effective for such low regularity problems ($u \in H^{5.5-\epsilon}$), and extrapolation can also help us to increase the accuracy of initial guess w_h in L^2 -norm, which would widen the scope of applicability of our method.

Table 13 Comparison of the number of iterations, CPU times (in seconds) and errors between the EXCMG method and classical multigrid methods with the Gauss-Seidel smoother. Here CPU_{w_h} denotes the computational time for constructing of the initial guess w_h .

	ϵ	V(1,1)			W(2,1)			EXCMG			
		Iters ¹	CPU	$\ u_h - u\ _\infty$	Iters ²	CPU	$\ u_h - u\ _\infty$	Iters ³	CPU	$\ u_h - u\ _\infty$	CPU_{w_h}
Exam 1	10^{-14}	16	46.1	8.61(-13)	12	47.6	8.39(-13)	8	12.9	8.49(-13)	0.6
Exam 2	10^{-14}	16	46.4	1.91(-12)	12	47.6	1.71(-12)	9	12.6	1.81(-12)	0.6
Exam 3	10^{-11}	13	41.5	7.83(-11)	9	39.4	7.22(-11)	8	11.8	2.40(-11)	0.6
Exam 4	10^{-09}	72	204.3	8.27(-10)	47	182.9	2.76(-10)	8	10.8	1.82(-10)	0.6
Exam 5	10^{-12}	14	42.8	1.77(-12)	10	41.3	1.75(-12)	9	13.8	1.81(-12)	0.6
Exam 6	10^{-13}	15	45.9	1.91(-12)	11	46.1	1.91(-12)	9	13.3	2.04(-12)	0.6

¹ Iters denotes the number of V-cycles required to reach the error tolerance ϵ .

² Iters denotes the number of W-cycles required to reach the error tolerance ϵ .

³ Iters denotes the number of CG iterations on the finest grid for EXCMG method.

Table 14 Comparison of the number of iterations, CPU times (in seconds) and errors between the EXCMG method and classical multigrid methods with the CG smoother.

	ϵ	V(1,1)			W(2,1)			EXCMG		
		Iters	CPU	$\ u_h - u\ _\infty$	Iters	CPU	$\ u_h - u\ _\infty$	Iters	CPU	$\ u_h - u\ _\infty$
Exam 1	10^{-14}	15	43.9	8.38(-13)	13	49.7	8.42(-13)	8	12.9	8.49(-13)
Exam 2	10^{-14}	15	43.3	1.76(-12)	13	49.0	1.73(-12)	9	12.6	1.81(-12)
Exam 3	10^{-11}	11	32.2	7.09(-11)	10	38.0	7.22(-11)	9	11.8	2.40(-11)
Exam 4	10^{-09}	101	295.3	1.74(-10)	30	115.8	1.71(-10)	8	10.8	1.82(-10)
Exam 5	10^{-12}	13	39.1	1.75(-12)	11	42.7	1.75(-12)	9	13.8	1.81(-12)
Exam 6	10^{-13}	14	40.9	1.97(-12)	11	42.4	1.95(-12)	9	13.3	2.04(-12)

5.2 Computational efficiency

In this subsection, we compare the efficiency of the our new EXCMG method with the efficiency of the classical V-cycle and W-cycle multigrid methods for above six examples. Results with Gauss-Seidel smoother are listed in table 13 while results with CG smoother are listed in table 14. In both tables, the number of iterations, computational time, the L^∞ -norm of the difference between the FD solution u_h and the exact solution u are provided. Moreover, the computational time for constructing of the initial guess w_h (line 6 in algorithm 1) is also listed in the last column of table 13, this step contains the extrapolation and quartic interpolation as described in section 4.3. By comparing the total computational time of the new EXCMG method with the classical V-cycle and W-cycle multigrid methods for all above six examples as listed in both table 13 and 14, one can easily find that the new EXCMG method needs the smallest time for all examples, and this is particularly true when using the unequal meshsizes in different directions, see example 4. Thus, the EXCMG method is much more efficient than the classical V-cycle and W-cycle multigrid methods. And from the last column in table 13, one can find that the computational time for constructing the initial guess w_h described in section 4.3 is 0.6 seconds for every example, which is very cheap, comparing to the total computational time.

Moreover, one can see from table 13 and 14 that there is only a few number of iterations are needed on the finest grid for every example in our EXCMG method, because that the initial guess w_h is already an extremely accurate approximation to the FD solution u_h . For example, from the last column of table 2, we see that the maximum error of the initial guess on the finest grid for example 1 is 4.15×10^{-12} , which implies that the number of significant figures of the approximation exceeds 10. Indeed, from table 1-12 we see that the extrapolated

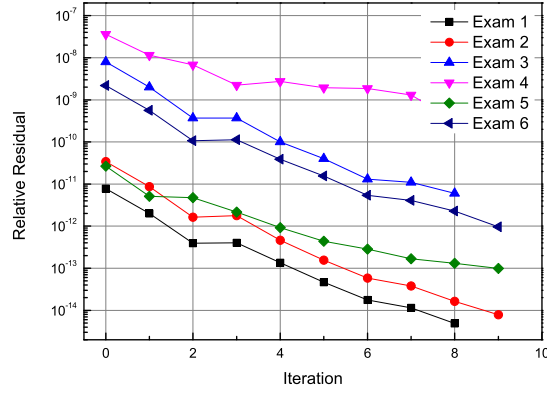


Fig. 4 Relative residual vs. the number of iterations on the finest grid.

value w_h served as an initial guess of the CG solver is a fifth-order approximation to the FD solution u_h in L^2 -norm, which is one order higher than the convergence order of the fourth-order difference solution u_h . Thus, the relative effect of how w_h approximates u_h becomes better when mesh is refined, and the number of iterations is reduced most significantly on the finest grid, see a more detailed discussion in [44].

Finally, we present the curve of the relative residual on the finest grid versus the number of iterations for the above six examples in Fig. 4. As we can see that the initial relative residual on the finest grid for each example is very small. And due to the high oscillations of the initial error as shown in section 4.4, the relative residual decreases by several orders of magnitude after only a few iterations, and then reaches a number that is less than the required tolerance.

6 Conclusions

In this work, we developed a new extrapolation cascadic multigrid (EXCMG) method combined with 19-point fourth-order compact difference scheme for solving the 3D Poisson equation on rectangular domains. The major advantage of the method is to use the Richardson extrapolation and tri-quartic Lagrange interpolation techniques for two numerical solutions on two-level of grids (current and previous grids) to obtain a fifth-order approximation w_h to the fourth-order FD solution u_h as the initial guess of the iterative solution on the next finer grid, which greatly reduces the iteration numbers. When the exact solution u is sufficiently smooth, a sixth-order extrapolated solution \tilde{u}_h on the fine grid can be obtained by using two fourth-order numerical solutions on two scale grids. Moreover, the gradient of solution ∇u_h can also be computed easily and efficiently through solving a series of tridiagonal linear systems resulting from the fourth-order compact FD discretization of the derivatives. Finally, numerical results show that our new extrapolation cascadic multigrid method is much more efficient comparing to the classical V-cycle and W-cycle multigrid method and it is particularly suitable for solving large scale problems.

The work presented in this paper is an extension of our previous work, which is based on the EXCMG method for the 3D elliptic problem with the linear FE discretization [44]. In the near future, we will extend our method to convection-diffusion equations, Helmholtz equations, biharmonic equations, and other related equations.

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